Vol. 79 (1991) ACTA PHYSICA POLONICA A No 5

# MULTIBAND $s$–$f$ MODEL FOR PSEUDOBINARY INTERMETALIC $Gd(Al_{1-x}Me_x)_2$ ALLOYS. II. Me = Pb, Bi, Si, Sb*

M. MATLAK AND J. ZIELIŃSKI

Institute of Physics, Silesian University, Uniwersytecka 4, 40-007 Katowice, Poland

*(Received August 9, 1990; in final version October 16, 1990)*

With the use of the formulae derived in the preceding paper we calculate the Curie temperature and the magnetic moment as functions of the concentration $x$ for $Gd(Al_{1-x}Me_x)_2$ (Me = Pb, Bi, Si, Sb) alloys. The agreement with the recent experimental data is relatively good.

PACS numbers: 75.30.Cr, 75.20.En

## 1. Introduction

Magnetically ordered intermetallic alloys with the general formula $Gd(Al_{1-x}Me_x)_2$ have been experimentally investigated in [1, 2] (Me = Cu, Ag, In, Pd, Sn) and very recently in [3–6] (Me = Pb, Bi, Si, Sb), where the dependence of the Curie temperature $T_c$ and the magnetic moment $M$ as functions of the concentration $x$ has been measured. The properties of the first group of alloys has been explained in [7] with the use of the multiband $s$–$f$ model. In the present paper we try to explain the properties of the second group of materials (Me = Pb, Bi, Si, Sb) using the formula for $T_c$ and $M$, derived in [7]. The above mentioned $s$–$f$ model contains all relevant exchange interactions which are of major importance in systems in which itinerant ($s$, $p$, $d$-electrons) and local electron magnetic moments ($4f$-electrons, $s = 7/2$ for Gd) are present. The mathematical structure of this model has been elucidated in [7], where it has also been indicated that values of only a few of many model parameters are significant for the fit to experimental data.

*Supported by CPBP 01.12.

## 2. Curie temperature and magnetic moment

We use here the same symbols denoting the model parameters as in [7]. For the bandwidths and their centers of gravity we reserve the symbols $W^{(a)}$ and $t^{(a)}$, respectively. The local $s$–$f$ coupling constant is denoted by $I^{(a)}$. The upper index $(a)$ numbers the bands coming from the elements Gd, Al or Me. Also in the case of Me = Pb, Bi, Sb, Si the parameters of Gd are completely irrelevant and only the parameters describing Al and Me are important. Actually, according to the equation (17) of [7], after introducing the number of electrons $n$ contributed by Me ($n = 4$ (Pb, Si), 5(Bi, Sb)) we can obtain the position of the chemical potential $\mu$. Because $\mu$ lies below the conducting bands ($5d$, $6s$) of Gd the contribution of the Gd parameters to the Curie temperature $T_c$ and magnetic moment $M$ (see Eqs. (15) and (16) of [7]) is zero. This fact reduces the number of relevant parameters of our model to that of Al and Me (Me = Pb, Bi, Si, Sb).

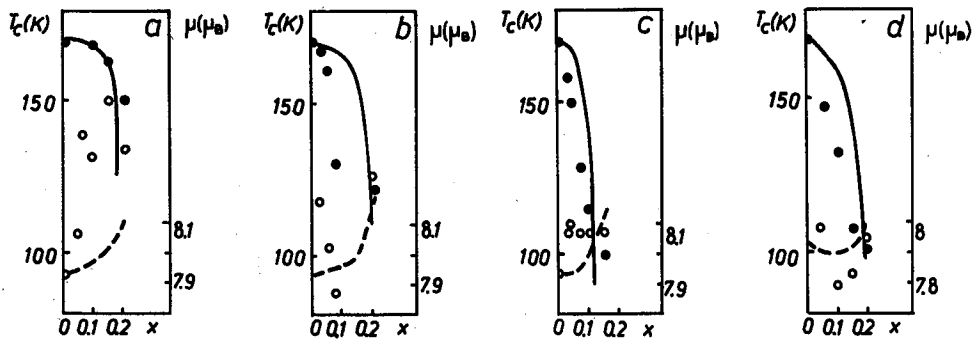


Fig. 1. The Curie temperature $T_c$ (left scale and continuous lines) and the magnetic moment $M$ (right scale and dashed lines) vs. concentration $x$ for $Gd(Al_{1-x}Me_x)_2$: (a) Me = Pb, (b) Me = Bi, (c) Me = Si, (d) Me = Sb. The parameters in eV: (Al) $I^{(3s)} = -0.093$, $t^{(3s)} = 0$, $W^{(3s)} = 4$, $I^{(3p)} = 0.027$, $t^{(3p)} = 2$, $W^{(3p)} = 3.5$; (Pb) $I^{(6s)} = 0.08$, $t^{(6s)} = 3$, $W^{(6s)} = 6.5$, $I^{(6p)} = 0.055$, $t^{(6p)} = 2.4$, $W^{(6p)} = 5$, $r_s = r_p = 1$, $n = 4$; (Bi) $I^{(6s)} = 0.06$, $t^{(6s)} = 1.8$, $W^{(6s)} = 6$, $I^{(6p)} = 0.05$, $t^{(6p)} = 2$, $W^{(6p)} = 5$, $r_s = r_p = 1$, $n = 5$; (Si) $I^{(3s)} = 0.02$, $t^{(3s)} = 0.5$, $W^{(3s)} = 4$, $I^{(3p)} = 0.03$, $t^{(3p)} = 3.4$, $W^{(3p)} = 3$, $r_s = r_p = 1$, $n = 4$; (Sb) $I^{(5s)} = -0.02$, $t^{(5s)} = 1.5$, $W^{(5s)} = 5$, $I^{(5p)} = -0.03$, $t^{(5p)} = 2$, $W^{(5p)} = 4$, $r_s = r_p = 1$, $n = 4$. The parameters $t^{(a)}$ are counted from the center of the $3s$ band of Al. The parameters for Gd are irrelevant. Full (blank) circles represent experimental data for $T_c$ (M).

In Figures 1(a)–(d) we show the dependence $T_c = T_c(x)$ and $M = M(x)$, calculated from the Eqs. (15), (17) and (16) of Ref. [7]. The parameters for Al are the same as in [7] and only the parameters for Me = Pb, Bi, Si, Sb has been chosen to get simultaneously the best possible fit for $T_c$ and $M$ of the experimental data for Me = Pb [3], Bi [4], Sb [5] and Si [6].

The agreement of our $T_c$ curves is relatively good, which is not the case for

the magnetic moment. This disagreement may be caused by the polycrystalline nature of the samples where the magnetization changes from one single crystal to the other (there is no homogeneous magnetization) but the Curie temperature remains the same for all the single crystals of the sample. This fact explains better agreement of our $T_c$ curves with the experimental data than that of the curves corresponding to the magnetic moment. It should be mentioned that parameters responsible for properties of Gd are irrelevant due to the specific position of the bands which corresponds to the physical situation [7]. The reasonable fit to the experimental data does not allow for pronounced variation of relevant parameters. However, their values meet physical reality.

## References

[1] A. Chełkowski, G. Wnętrzak, *Acta Phys. Pol.* **A68**, 485 (1985).

[2] A. Chełkowski, G. Wnętrzak, *J. Less-Common Met.* **111**, 157 (1985).

[3] G. Chełkowska, A. Chełkowski, to be published.

[4] J. Jarosz, A. Ślebarski, A. Chełkowski, to be published in *J. Phys. C* (1990).

[5] J. Jarosz, A. Ślebarski, to be published.

[6] G. Chełkowska, A. Chełkowski, to be published.

[7] M. Matlak, J. Zieliński, *Acta Phys. Pol.* **A78**, 929 (1990).